**Method**

* We simulated different SAMs forming on a gold surface through our AROMODEL script. We split our simulations into different classes of molecules:
  + Oligo ethylene glycols (OEGs)
  + …
* We formed different molecules’ data files (.xyz files) through OpenBabel
* Ran DFT corrections through ORCA
* Created a LAMMPS file
* Simulated a cooling

**Analysis**

* Analyzed the max heights of every molecule for a given class
* Quantified helixing through the tangent correlation function